

Dynamical Mean-Field Study of Local Pairing Interaction Mediated by Spin and Orbital Fluctuations in Iron Pnictide Superconductors

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We investigate the two-orbital Hubbard model, which reproduces the electron and hole Fermi surfaces in the iron pnictide superconductors, in the presence of the Jahn-Teller electron-phonon coupling by using the dynamical mean-field theory. When the intra- and inter-orbital Coulomb interactions, U and U' , increase with $U = U'$, both the local spin and orbital susceptibilities, χ_s and χ_o , increase with $\chi_s = \chi_o$ because of the spin-orbital symmetry. Due to the Hund's rule coupling J , χ_s is enhanced and dominates over χ_o resulting in the repulsive local pairing interaction $V_{loc} > 0$, while due to the electron-phonon coupling g , χ_o is enhanced and dominates over χ_s resulting in the attractive one $V_{loc} < 0$ which induces the intra-orbital s -wave pairing. Remarkably, V_{loc} is weakly dependent on doping and can be attractive for heavily electron-doped regime where the superconductivity is observed without Fermi surface nesting.

KEYWORDS: iron pnictide superconductor, multi-orbital system, Jahn-Teller electron-phonon coupling, orbital fluctuation, magnetic fluctuation, dynamical mean-field theory

The iron pnictide superconductors exhibit the common feature of phase diagrams, where parent compounds show the tetragonal-orthorhombic structural transition and the stripe-type antiferromagnetic (AFM) transition both of which are suppressed by carrier doping x resulting in the high- T_c superconductivity.^{1,2)} When approaching the AFM transition, the AFM fluctuation observed by the NMR experiments³⁾ is found to be enhanced, while, when approaching the structural transition, the d_{xz} - d_{yz} ferro-orbital (FO) fluctuation (or the $O_{x^2-y^2}$ ferroquadrupole fluctuation)⁴⁾ responsible for the softening of the elastic constant C_{66} observed by the ultrasonic experiments^{5,6)} is found to be enhanced. Correspondingly, two distinct s -wave pairings: the s_{\pm} -wave with sign change of the order parameter between the hole and the electron Fermi surfaces (FSs) mediated by the AFM fluctuation^{7,8)} and the s_{++} -wave without the sign change mediated by the FO fluctuation^{9,10)} and by the antiferro-orbital (AFO) fluctuation¹¹⁾ which is also responsible for the softening of C_{66} through the two-orbital process,¹²⁾ were proposed.

Recent experiments have revealed that the high- T_c superconductivity is realized even in the case with heavily electron-doped compounds such as $R\text{FeAsO}_{1-x}\text{H}_x$ ($R=\text{Sm, Ce, La}$)¹³⁻¹⁵⁾ up to $x \sim 0.5$ and $\text{A}_x\text{Fe}_2\text{Se}_2$ ($\text{A}=\text{K, Cs, Rb}$)^{16,17)} where the large electron FSs are observed without the hole FSs. In this case, the mechanisms based on the AFM^{7,8)} and the AFO¹¹⁾ fluctuations, which are enhanced due to the nesting between the electron and hole FSs, seem to be insufficient for explaining the superconductivity. As for the mechanism based on the FO fluctuation⁹⁾ which is enhanced due to the coupling between the d_{xz} - d_{yz} orbital fluctuation and the orthorhombic phonon, the superconductivity does not need the FS nesting effect but is restricted near the tetragonal-orthorhombic structural transition with small x within

the random phase approximation (RPA).

Generally, in the magnetic fluctuation mechanism, the pairing interaction $V(\mathbf{q})$ with wavevector \mathbf{q} is repulsive and then the strong \mathbf{q} -dependence of $V(\mathbf{q})$ realized near the magnetic ordered phase is crucial for the superconductivity. On the other hand, in the orbital fluctuation mechanism, $V(\mathbf{q})$ is attractive and then the strong \mathbf{q} -dependence of $V(\mathbf{q})$ realized near the orbital ordered phase is not necessary for the superconductivity. When the local component of the orbital fluctuation is relatively larger than that of the magnetic fluctuation, the local component of the pairing interaction V_{loc} , which is nothing but the \mathbf{q} -averaged value of $V(\mathbf{q})$, becomes attractive and induces the s_{++} -wave pairing, even far away from the ordered phases.

In this letter, we investigate the local pairing interaction V_{loc} mediated by the spin and orbital fluctuations by using the dynamical mean-field theory (DMFT)¹⁸⁾ which becomes exact in infinite dimensions ($d = \infty$) and enables us to sufficiently include the local correlation effect beyond the RPA. We employ the two-orbital Hubbard model,^{19,20)} which reproduces the electron and hole FSs in the iron pnictides, in the presence of the coupling between the orbital fluctuation and the Jahn-Teller (JT) phonon corresponding to the orthorhombic mode responsible for the softening of C_{66} as discussed in the previous work.^{9,10)} Although the present model is a simplified version of the multi-orbital electron-phonon models for the iron pnictides,^{9-12,21)} the essential feature of the local magnetic and orbital fluctuations, which is crucial for determining V_{loc} , is expected to be well described.

Our model Hamiltonian is given by

$$H = H_0 + H_{\text{int}} + H_{\text{ph}} + H_{\text{el-ph}} \quad (1)$$

with the kinetic part of the Hamiltonian:

$$H_0 = \sum \left(d_{\mathbf{k}1\sigma}^\dagger d_{\mathbf{k}2\sigma}^\dagger \right) \hat{H}_{\mathbf{k}} \begin{pmatrix} d_{\mathbf{k}1\sigma} \\ d_{\mathbf{k}2\sigma} \end{pmatrix}, \quad \hat{H}_{\mathbf{k}} = \begin{pmatrix} \epsilon_{\mathbf{k}1} & \epsilon_{\mathbf{k}12} \\ \epsilon_{\mathbf{k}12} & \epsilon_{\mathbf{k}2} \end{pmatrix} \quad (2)$$

where $d_{\mathbf{k}l\sigma}$ is the annihilation operator for a Fe 3d electron with the wavevector \mathbf{k} and the spin σ in the orbital $l = 1, 2 (= d_{xz}, d_{yz})$, and the energies $\epsilon_{\mathbf{k}l}$ and $\epsilon_{\mathbf{k}12}$ are determined so as to reproduce the electron and hole FSs in the iron pnictides.¹⁹⁾ The Coulomb interaction part H_{int} includes the intra- and inter-orbital direct terms U and U' , the Hund's rule coupling J and the pair transfer J' . For simplicity, we assume the relations $U = U' + 2J$ and $J = J'$ which are satisfied in the isolated atom but not generally in the crystal.^{22,23)} The phonon and the electron-phonon interaction parts are given by

$$H_{\text{ph}} + H_{\text{el-ph}} = \sum_i \omega_0 b_i^\dagger b_i + g \sum_i (b_i + b_i^\dagger) \tau_{zi}, \quad (3)$$

where b_i is the annihilation operator for a JT phonon at site i with the frequency ω_0 , which is coupled to the longitudinal orbital fluctuation, $\tau_{zi} = \sum_\sigma (n_{i1\sigma} - n_{i2\sigma})$ with $n_{i1\sigma} = d_{i1\sigma}^\dagger d_{i1\sigma}$, through the electron-phonon coupling g .

To solve the model eq.(1), we use the DMFT¹⁸⁾ in which the lattice model is mapped onto an impurity Anderson model embedded in an effective medium which is determined so as to satisfy the self-consistency condition

$$[\hat{G}^{-1}(z) - \hat{\Sigma}(z)]^{-1} = \frac{1}{N} \sum_{\mathbf{k}} [z - \hat{H}_{\mathbf{k}} - \hat{\Sigma}(z)]^{-1}, \quad (4)$$

where $\hat{\Sigma}(z)$ and $\hat{G}(z)$ are the 2×2 matrix representations of the impurity (local) self-energy and the bare impurity Green's function, respectively, and z is the complex frequency.

We write the effective pairing interaction for the spin-singlet state mediated by the spin and charge-orbital fluctuations in the 4×4 matrix representation as²⁴⁾

$$\hat{V}(\mathbf{q}, z) = \frac{3}{2} \hat{\Gamma}_s(z) \hat{\chi}_s(\mathbf{q}, z) \hat{\Gamma}_s(z) - \frac{1}{2} \hat{\Gamma}_c(z) \hat{\chi}_c(\mathbf{q}, z) \hat{\Gamma}_c(z) + \frac{1}{2} (\hat{\Gamma}_s^{(0)} + \hat{\Gamma}_c^{(0)}), \quad (5)$$

where $\hat{\Gamma}_{s(c)}(z)$ is the local irreducible spin (charge-orbital) vertex in which only the external frequency (z) dependence is considered as a simplified approximation.²⁵⁾ The corresponding bare vertex is given by: $[\Gamma_{s(c)}^{(0)}]_{ll'uu} = U(U - 2g^2 D(z))$, $[\Gamma_{s(c)}^{(0)}]_{ll'uv} = U'(-U' + 2J)$, $[\Gamma_{s(c)}^{(0)}]_{ll'vv} = J(2U' - J + 2g^2 D(z))$ and $[\Gamma_{s(c)}^{(0)}]_{ll'vu} = J'(J')$ with the bare phonon Green's function $D(z) = 2\omega_0/(\omega_0^2 - z^2)$, where $l' \neq l$ and the other matrix elements are 0.^{22,23)} Within the DMFT, the spin (charge-orbital) susceptibility can be expressed as $\hat{\chi}_{s(c)}(\mathbf{q}, z) = [\hat{\chi}_0(\mathbf{q}, z)^{-1} - (+)\hat{\Gamma}_{s(c)}(z)]^{-1}$, where $\hat{\chi}_0(\mathbf{q}, i\omega) = -T \sum_{\mathbf{k}\epsilon} \hat{G}(\mathbf{k} + \mathbf{q}, i\epsilon + i\omega) \hat{G}(\mathbf{k}, i\epsilon)$ with the lattice Green's function $\hat{G}(\mathbf{k}, z) = [z - \hat{H}_{\mathbf{k}} - \hat{\Sigma}(z)]^{-1}$, and the local vertex can be expressed as $\hat{\Gamma}_{s(c)}(z) = \hat{\chi}_0^{-1}(z) - \hat{\chi}_{s(c)}^{-1}(z)$, where $\hat{\chi}_0(i\omega) = -T \sum_{\epsilon} \hat{G}(i\epsilon + i\omega) \hat{G}(i\epsilon)$ with the local (impurity) Green's function $\hat{G}(z) = [\hat{G}^{-1}(z) - \hat{\Sigma}(z)]^{-1}$. When we replace $\hat{\Gamma}_{s(c)}(z)$ with $\hat{\Gamma}_s^{(0)}$ and neglect $\hat{\Sigma}(z)$, eq. (5) yields the RPA result of $\hat{V}(\mathbf{q}, z)$.²¹⁻²⁴⁾ Therefore, eq.(5) is a straightforward extension of the RPA result of $\hat{V}(\mathbf{q}, z)$ to include the vertex and the self-energy corrections within the DMFT without double

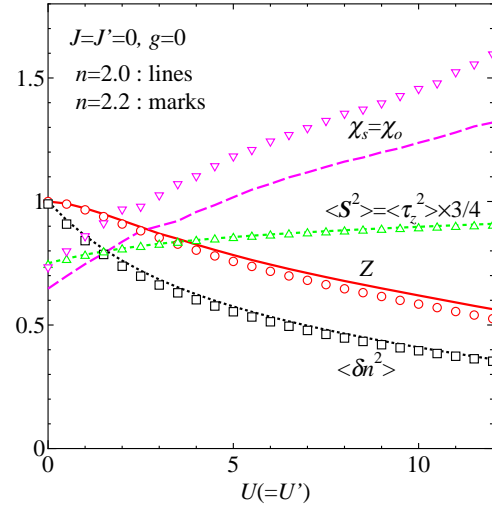


Fig. 1. (Color online) $U(=U')$ dependence of Z , $\langle S^2 \rangle$, $\langle \delta n^2 \rangle$, χ_s and χ_o with $J = J' = g = 0$ for $n = 2$ (lines) and $n = 2.2$ (marks).

counting.

The superconductivity can be examined by solving the Eliashberg equation with $\hat{V}(\mathbf{q}, z)$ given in eq.(5) where the 1st and 2nd terms of r.h.s. yield \mathbf{k} -dependent anomalous self-energies (or gap functions) which includes $1/d$ corrections for the DMFT.¹⁸⁾ In this letter, we focus only on the intra-orbital part of the local pairing interaction $V_{\text{loc}} \equiv [\hat{V}(z=0)]_{llll}$ with $\hat{V}(z) = \frac{1}{N} \sum_{\mathbf{q}} \hat{V}(\mathbf{q}, z) = \frac{3}{2} \hat{\Gamma}_s(z) \hat{\chi}_s(z) \hat{\Gamma}_s(z) - \frac{1}{2} \hat{\Gamma}_c(z) \hat{\chi}_c(z) \hat{\Gamma}_c(z) + \frac{1}{2} (\hat{\Gamma}_s^{(0)} + \hat{\Gamma}_c^{(0)})$, as it is the most dominant contribution for the s_{++} -wave pairing due to the orbital fluctuation.^{9,10)}

In the actual calculations with the DMFT, we solve the effective impurity Anderson model coupled to the JT phonon by using the exact diagonalization (ED) method for a finite-size cluster to obtain the local quantities such as $\hat{\Sigma}(z)$ and $\hat{\chi}_{s(c)}(z)$ at $T = 0$, where we set the site number $N_s = 4 - 6$ and the cutoff of the phonon number $N_b = 20$.^{26,27)} The tight-binding parameters are set to be the same in Ref.¹⁹⁾ where the total band width is $W = 12$, and we set the phonon frequency $\omega_0 = 0.01W$. Using the ED method, we calculate the several physical quantities as follows: the renormalization factor corresponding to the inverse effective mass $Z = (1 - \frac{d\Sigma(z)}{dz}|_{z=0})^{-1} = (m^*/m)^{-1}$, the local charge, spin and orbital fluctuations $\langle \delta n^2 \rangle$ with $\delta n = n - \langle n \rangle$, $\langle S^2 \rangle$ with $S = \frac{1}{2} \sum_l \sum_{\alpha\beta} d_{l\alpha}^\dagger \sigma_{\alpha\beta} d_{l\beta}$ and $\langle \tau_z^2 \rangle$, and the local spin and orbital susceptibilities $\chi_s = 4\langle \langle S_z | S_z \rangle \rangle|_{z=0}$ and $\chi_o = \langle \langle \tau_z | \tau_z \rangle \rangle|_{z=0}$, together with the intra-orbital local pairing interaction V_{loc} mentioned above.

Fig. 1 shows the several physical quantities mentioned above as functions of $U(=U')$ with $J = J' = g = 0$ at half-filling $n = 2$ and away from half-filling $n = 2.2$. When the electron correlation increases with $U = U'$, Z and $\langle \delta n^2 \rangle$ decrease while $\langle S^2 \rangle$ and $\langle \tau_z^2 \rangle$ increase with $\langle S^2 \rangle = \frac{3}{4} \langle \tau_z^2 \rangle$ as the double-occupancy probabilities take the same value: $\langle n_{l\uparrow} n_{l\downarrow} \rangle = \langle n_{l\uparrow} n_{l'\downarrow} \rangle = \langle n_{l\uparrow} n_{l'\uparrow} \rangle$ with $l \neq l'$ because of the spin-orbital symmetry.²⁷⁾ Correspondingly, χ_s and χ_o increase with $\chi_s = \chi_o$ while the charge susceptibility decreases (not shown) with increasing U .

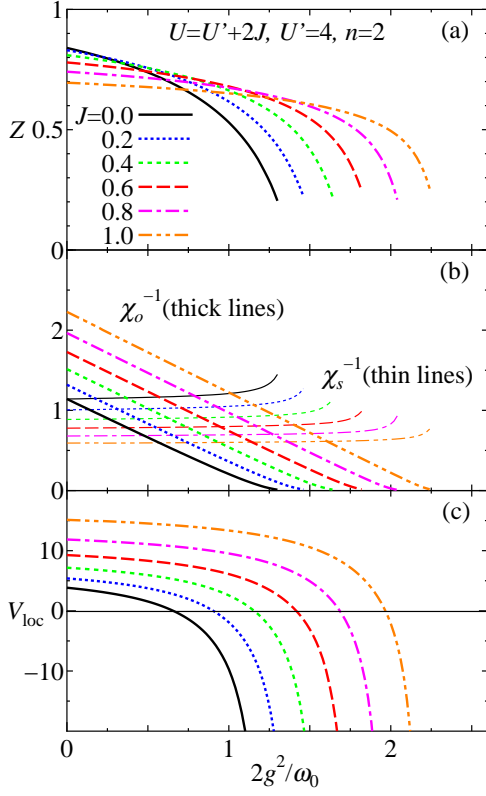


Fig. 2. (Color online) $2g^2/\omega_0$ dependence of Z (a), $\chi_{s(o)}^{-1}$ (b) and V_{loc} (c) for several values of $J(=J')$ with $U' = 4$ and $n = 2$.

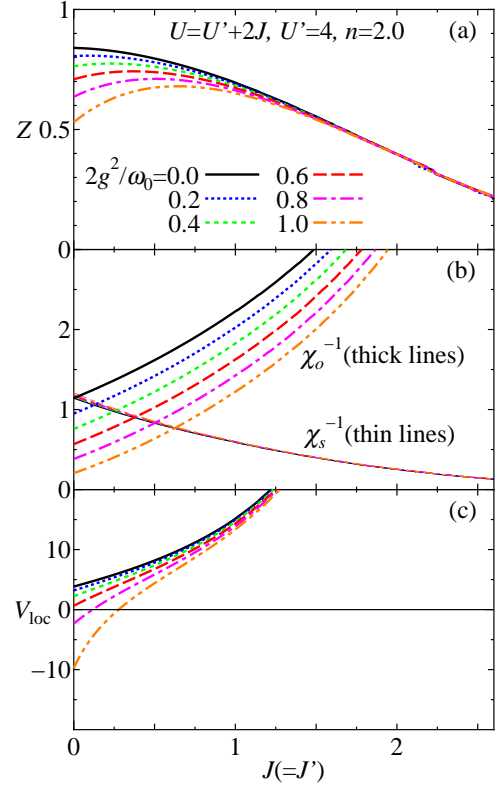


Fig. 3. (Color online) J dependence of Z (a), χ_s and χ_o (b) and V_{loc} (c) for several values of $2g^2/\omega_0$ with $U' = 4$ and $n = 2$.

For $n = 2$, we also observe the Mott metal-insulator transition at a critical interaction $U_c(= U'_c) \sim 2.5W$, where $Z = 0$ for $U > U_c$, while when $U \rightarrow U_c$ for $U < U_c$, $Z \rightarrow 0$ and $\chi_s = \chi_o \rightarrow \infty$ (not shown), as previously observed in the multi-orbital Hubbard model.²⁸⁾ For $n = 2.2$, the U dependence of the physical quantities is almost similar to that for $n = 2$ as shown in Fig. 1, except for the Mott transition which is observed exclusively for integer fillings.²⁸⁾ We note that, although the \mathbf{q} dependence of $\hat{\chi}_s(\mathbf{q}, z)$ largely depends on doping responsible for the Fermi surface nesting, the \mathbf{q} -averaged value, i. e., the local susceptibility $\hat{\chi}_s(z)$ is weakly dependent on doping.

Next, we consider the effects of the Hund's rule coupling $J(=J')$ and the JT electron-phonon coupling g . In Figs. 2 (a)-(c), Z , $\chi_{s(o)}^{-1}$ and V_{loc} are plotted as functions of $2g^2/\omega_0$ for several values of J with $U' = 4$ and $n = 2$. When $2g^2/\omega_0$ increases, Z decreases with increasing χ_o due to the strong orbital-lattice coupling effect, while χ_s slightly decreases. Correspondingly, V_{loc} decreases with increasing $2g^2/\omega_0$ and finally becomes negative where the attractive term due to χ_o dominates over the repulsive term due to χ_s (see eq.(5)). Then, the intra-orbital s -wave (s_{++} -wave) pairing is expected to be realized in the intermediate coupling regime where $V_{\text{loc}} < 0$ and $Z = 1/2 \sim 1/3$. In the strong coupling regime, we also observe the bipolaronic transition at a critical coupling g_c where $Z \rightarrow 0$ with $g \rightarrow g_c$ together with $\chi_o \rightarrow \infty$ and $V_{\text{loc}} \rightarrow \infty$, although it is difficult to obtain a fully convergent solution with $Z \sim 0$. The effect of J enhances

χ_s while suppresses χ_o (see also Fig. 3).

Figs. 3 (a)-(c) show the J dependence of Z , $\chi_{s(o)}^{-1}$ and V_{loc} for several values of $2g^2/\omega_0$ with $U' = 4$ and $n = 2$. When J increases, Z monotonically decreases for $2g^2/\omega_0 = 0$ while it shows a maximum at $J \sim 2g^2/\omega_0$ for $2g^2/\omega_0 \neq 0$. $\chi_s(\chi_o)$ increases (decreases) with increasing J resulting in a crossover between the following two regimes: $J \lesssim 2g^2/\omega_0$ with $\chi_s < \chi_o$ and $J \gtrsim 2g^2/\omega_0$ with $\chi_s > \chi_o$. Then, the large effective mass $m^*/m = Z^{-1} \gg 1$ is observed in the two distinct regimes with $J \ll 2g^2/\omega_0$ ($J \gg 2g^2/\omega_0$) where $\chi_o(\chi_s)$ dominates over $\chi_s(\chi_o)$ due to the strong coupling (correlation) effect, while the moderate effective mass $m^*/m = Z^{-1} = 2 \sim 3$ is observed in the intermediate regime with $J \sim 2g^2/\omega_0$ where χ_s and χ_o , both of which are largely enhanced by $U(=U')$ as shown in Fig. 1, compete to each other resulting in a maximum of Z as a fully non-perturbative effect. This intermediate regime with χ_o being a little larger than χ_s is responsible for the s_{++} -wave pairing with $V_{\text{loc}} < 0$ and seems to be consistent with the iron-pnictide superconductors where both the spin and orbital fluctuations are large while the renormalization of the band width is moderate $Z = 1/2 \sim 1/3$.²⁾

Finally, we study the doping dependence of V_{loc} . In Fig. 4, we plot V_{loc} as a function of n for several values of $2g^2/\omega_0$ with $U' = 4$ and $J = 0.4$. For small $2g^2/\omega_0$, V_{loc} is repulsive as χ_s dominates over χ_o . When $2g^2/\omega_0$ increases, χ_o increases and then dominates over χ_s resulting in $V_{\text{loc}} < 0$ as shown in Fig. 2 (c) for $n = 2$. Remarkably, V_{loc} is weakly dependent on n and can be attractive

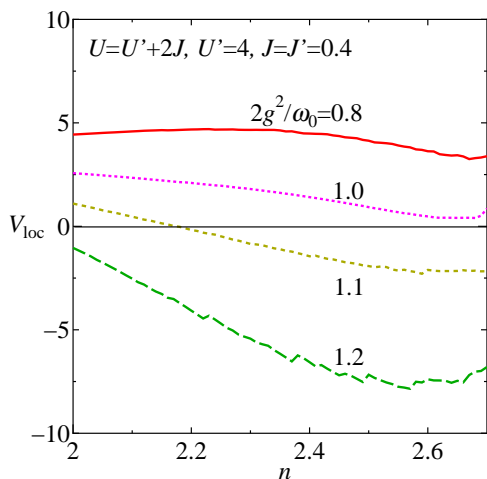


Fig. 4. (Color online) n dependence of V_{loc} for several values of $2g^2/\omega_0$ with $U' = 4$ and $J = J' = 0.4$.

even far away from half-filling, where the s_{++} -wave superconductivity is expected to be realized without the nesting between the electron and hole FSs as recently observed in the heavily electron-doped compounds.^{13–17}

In summary, we have investigated the local pairing interaction V_{loc} mediated by the spin and orbital fluctuations in the two-orbital Hubbard model for iron pnictides by using the DMFT+ED method which enables us to sufficiently include the local correlation effects due to the Coulomb and JT electron-phonon interactions beyond the RPA. It has been found that V_{loc} is weakly dependent on doping and becomes attractive in the intermediate regime with $J \lesssim 2g^2/\omega_0$ where the local orbital susceptibility is a little larger than the local spin susceptibility and the band width renormalization is moderate $1/2 \sim 1/3$. The result is responsible for the s_{++} -wave pairing even far away from the half-filling without Fermi surface nesting and seems to be consistent with the high- T_c superconductivity observed in the heavily electron-doped compounds.^{13–17}

Based on the present study, we can calculate the \mathbf{q} -dependent spin (charge-orbital) susceptibility $\chi_{s(c)}(\mathbf{q}, z)$ and determine the instability towards the ordered phase when the corresponding susceptibility diverges. Preliminary results shows that the stripe-type AFM observed for $J \gtrsim 2g^2/\omega_0$ is largely suppressed as compared to the RPA result due to the strong correlation effect within the DMFT while the suppression of the FO observed for $J \lesssim 2g^2/\omega_0$ is not so large. We also obtain some results for the superconductivity by solving the Eliashberg equation and find that the s_{\pm} -wave occurs near the AFM while the s_{++} -waves occur near the FO, where the s_{++} -region is qualitatively consistent with the $V_{\text{loc}} < 0$ region shown in this letter but expands to a rather smaller value of $2g^2/\omega_0$. Detailed calculations for the present model, together with those for a more realistic 5-orbital model, are now under way.

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